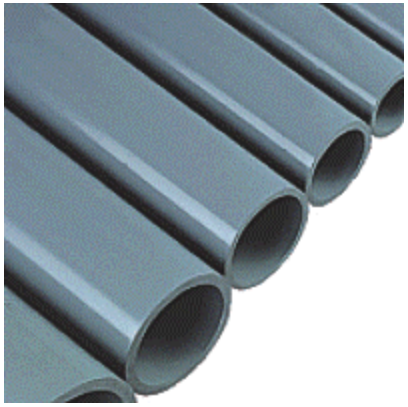
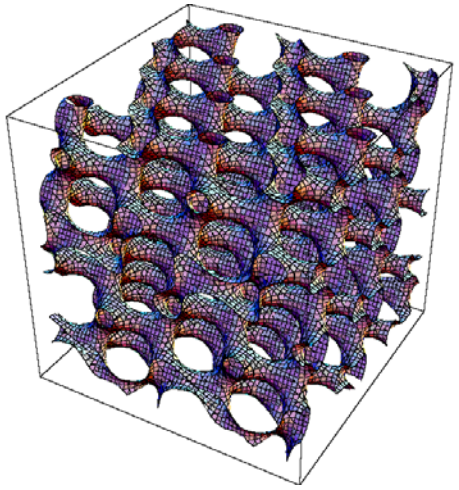
Simulating Polymer Materials with Fields

Glenn H. Fredrickson, UC Santa Barbara, DMR-0312097

Polymers are key ingredients in many soft material formulations including plastics, personal care products, and processed foods. Computer simulations of these materials are difficult, because structure is present on scales from 10^{-1}-10^{4} nm. We have found that the use of continuous chemical potential *fields*, rather than atomic coordinates, provides a powerful framework to carry out computer simulations o these "complex fluids". These field-based simulation techniques can be used to discover fascinating structures in exciting new types of materials, such as the ABC triblock copolymer at right.





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Education:

Three current graduate students (Deena Patel, August Bosse, and Alfredo Alexander-Katz), and four postdocs (Francois Drolet, Venkat Ganesan, Scott Sides, Ellen Reister) have contributed to developing field-based computer simulation techniques. Venkat is now an Assistant Prof. of Chem. Engr. at the U. of Texas at Austin. Francois Drolet is a Scientist at PAPRICAN, the Pulp and Paper Institute of Canada. Our group is also working closely with graduate students Matthew Hammond, Vikram Khanna, and Alex Hexemer in Prof. Kramer's group at UCSB on simulations relevant to their experimental projects.